LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.522	495	499	520	rBV2	47763	156726	8.08%	1.009%
2	5.216	613	617	648	rBV	745258	1594362	82.18%	10.262%
3	6.892	898	902	913	rBV	937017	1498258	77.22%	9.643%
4	6.981	913	917	934	rVB	1178459	1940158	100.00%	12.487%
5	7.322	971	975	987	rBV	243936	342872	17.67%	2.207%
6	7.557	1010	1015	1033	rBV	976463	1329996	68.55%	8.560%
7	8.239	1127	1131	1150	rBV	630908	978217	50.42%	6.296%
8	9.351	1316	1320	1343	rBV	303244	471177	24.29%	3.033%
9	11.133	1617	1623	1640	rBV	1442707	1896148	97.73%	12.204%
10	11.827	1737	1741	1759	rBV	119363	176010	9.07%	1.133%
11	12.168	1795	1799	1806	rBV2	373911	480845	24.78%	3.095%
12	13.027	1940	1945	1950	rBB2	22496	26109	1.35%	0.168%
13	13.468	2015	2020	2041	rBV	563874	887443	45.74%	5.712%
14	13.798	2071	2076	2084	rBV2	20425	36080	1.86%	0.232%
15	14.568	2203	2207	2223	rVB	259840	421097	21.70%	2.710%
16	15.592	2376	2381	2389	rBV	93809	121560	6.27%	0.782%
17	16.303	2498	2502	2510	rBV4	24454	49587	2.56%	0.319%
18	16.392	2514	2517	2525	rVB	76535	102356	5.28%	0.659%
19	16.698	2564	2569	2579	rBV	100805	147091	7.58%	0.947%
20	16.939	2606	2610	2616	rVB	1048599	1180876	60.86%	7.600%
21	18.203	2821	2825	2834	rBV4	28541	53789	2.77%	0.346%
22	18.286	2834	2839	2845	rBV2	297279	415646	21.42%	2.675%
23	19.321	3010	3015	3020	rBV	199747	223175	11.50%	1.436%
24	19.427	3028	3033	3039	rVB	237182	256659	13.23%	1.652%
25	19.562	3052	3056	3060	rBV	54476	78207	4.03%	0.503%
26	19.597	3060	3062	3073	rVB3	22555	32682	1.68%	0.210%
27	19.850	3102	3105	3110	rBV	39551	44788	2.31%	0.288%
28	19.909	3112	3115	3119	rVV	48217	56066	2.89%	0.361%
29	19.956	3119	3123	3134	rVV	254212	370236	19.08%	2.383%
30	20.056	3136	3140	3146	rVB4	16306	23544	1.21%	0.152%
31	20.650	3235	3241	3248	rBV9	9435	21356	1.10%	0.137%
32	20.750	3253	3258	3261	rBV3	15149	21830	1.13%	0.141%
33	21.156	3320	3327	3337	rBV4	22289	60076	3.10%	0.387%
34	21.485	3379	3383	3393	rVB3	19233	42090	2.17%	0.271%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

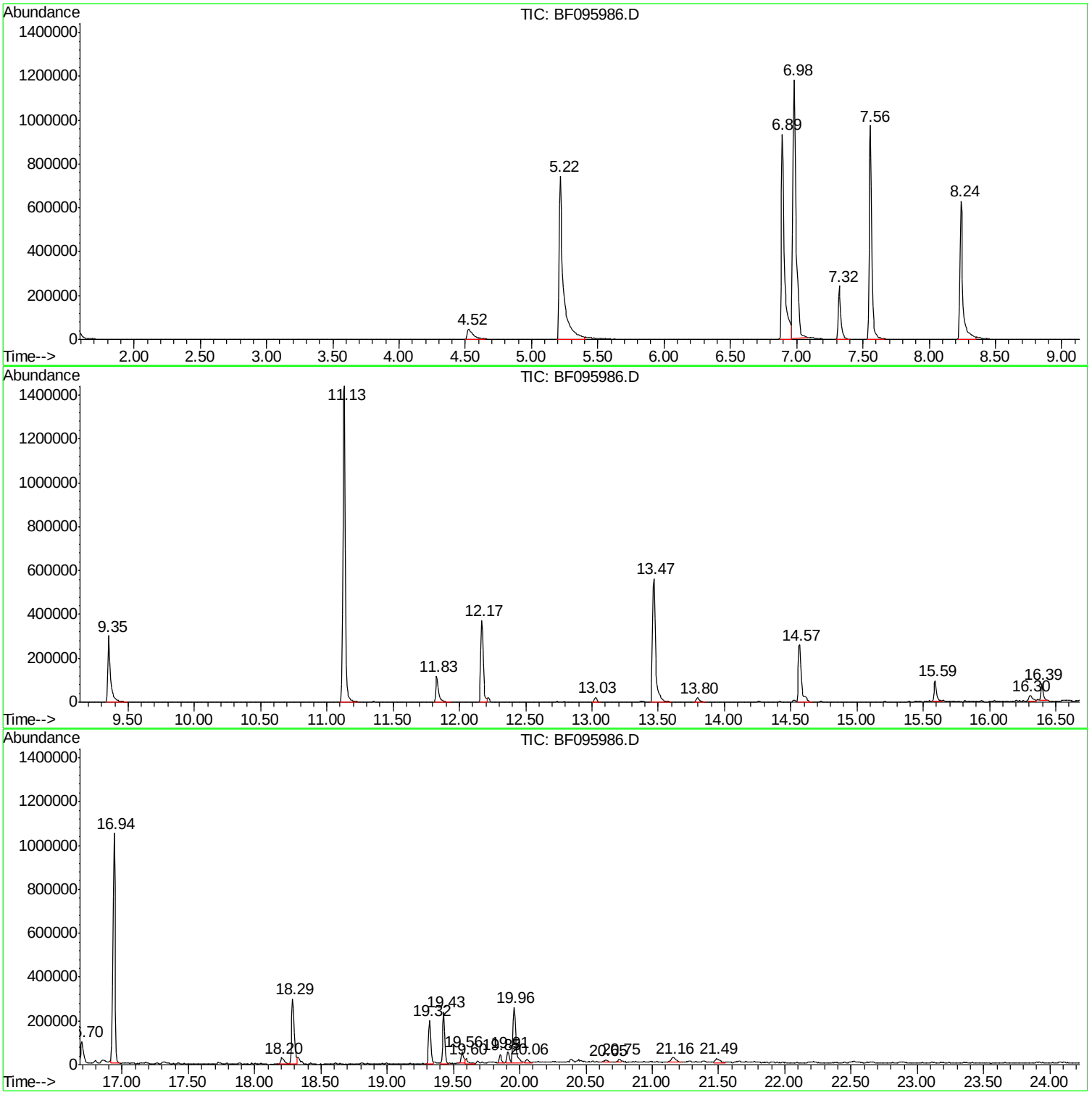
Sum of corrected areas: 15537112

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
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Sample : I3688-13
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

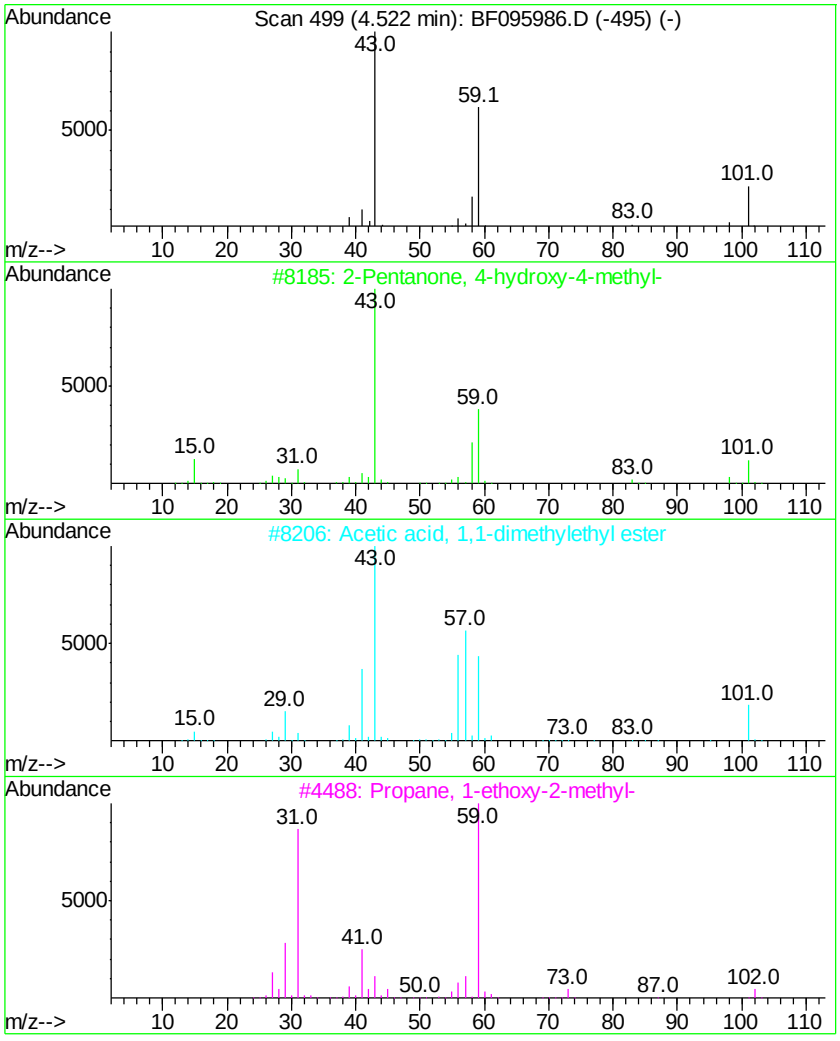
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

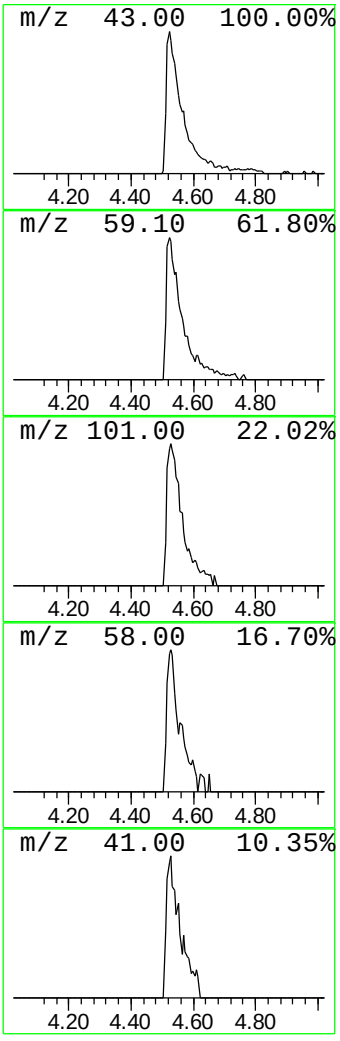
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	9.14 ng	156726	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

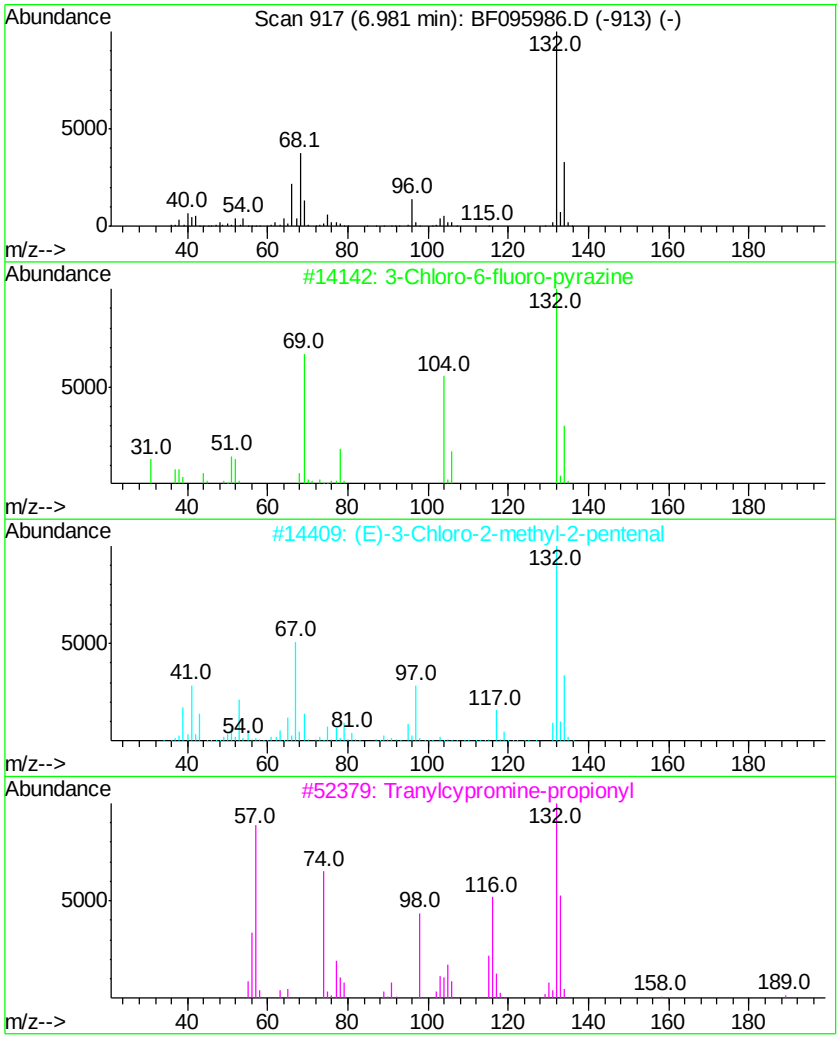
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

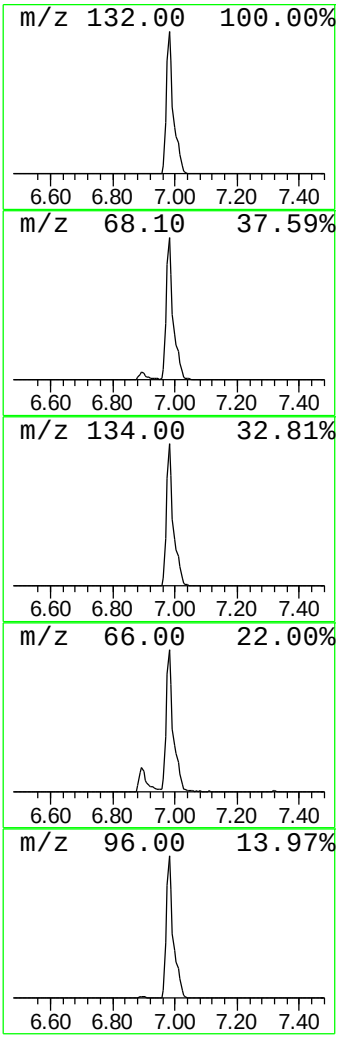
****

Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	113.17 ng	1940160	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

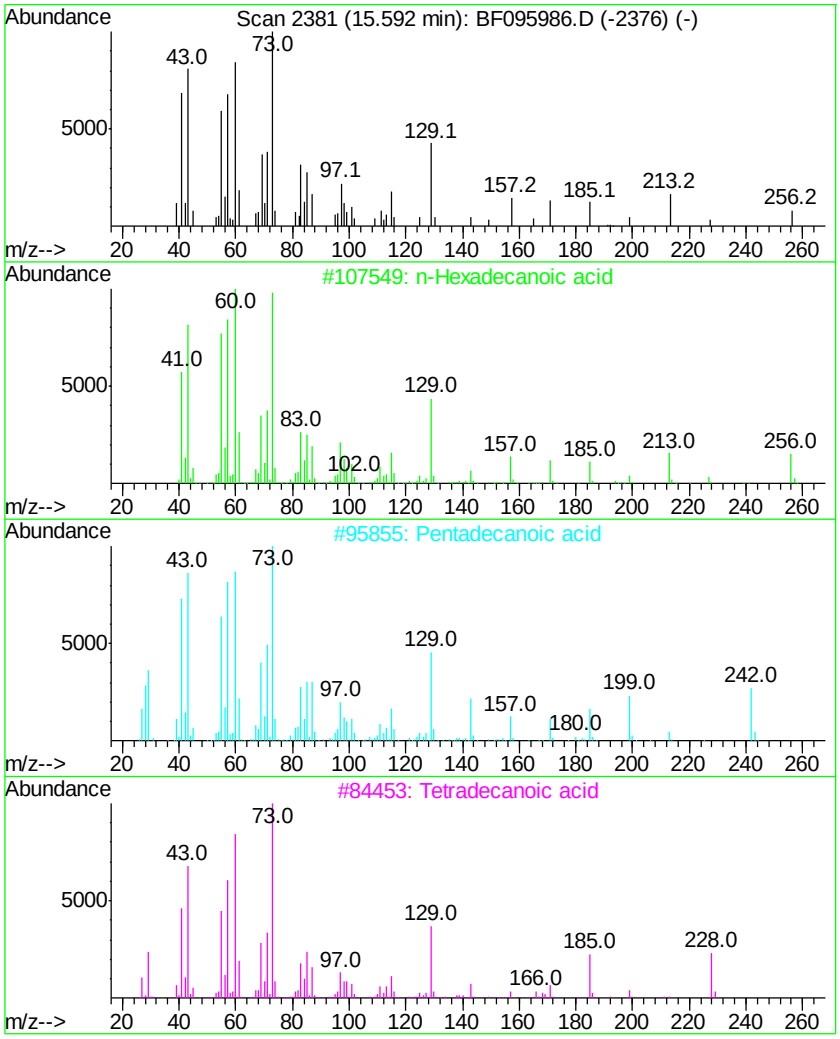
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

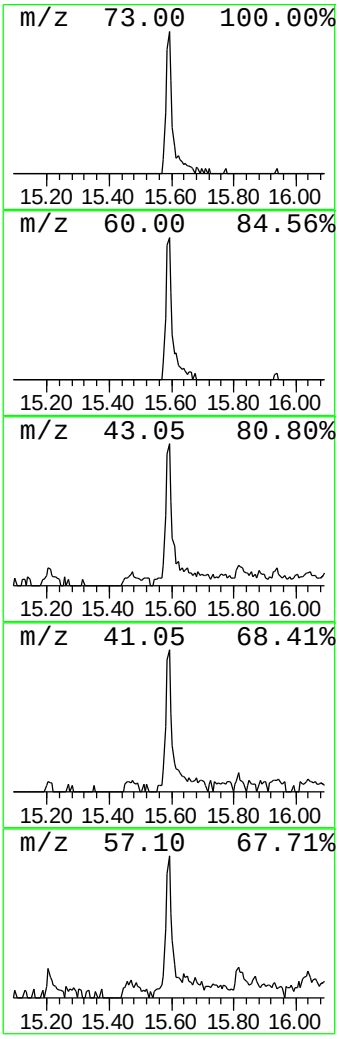
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	5.77 ng	121560	Phenanthrene-d10	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

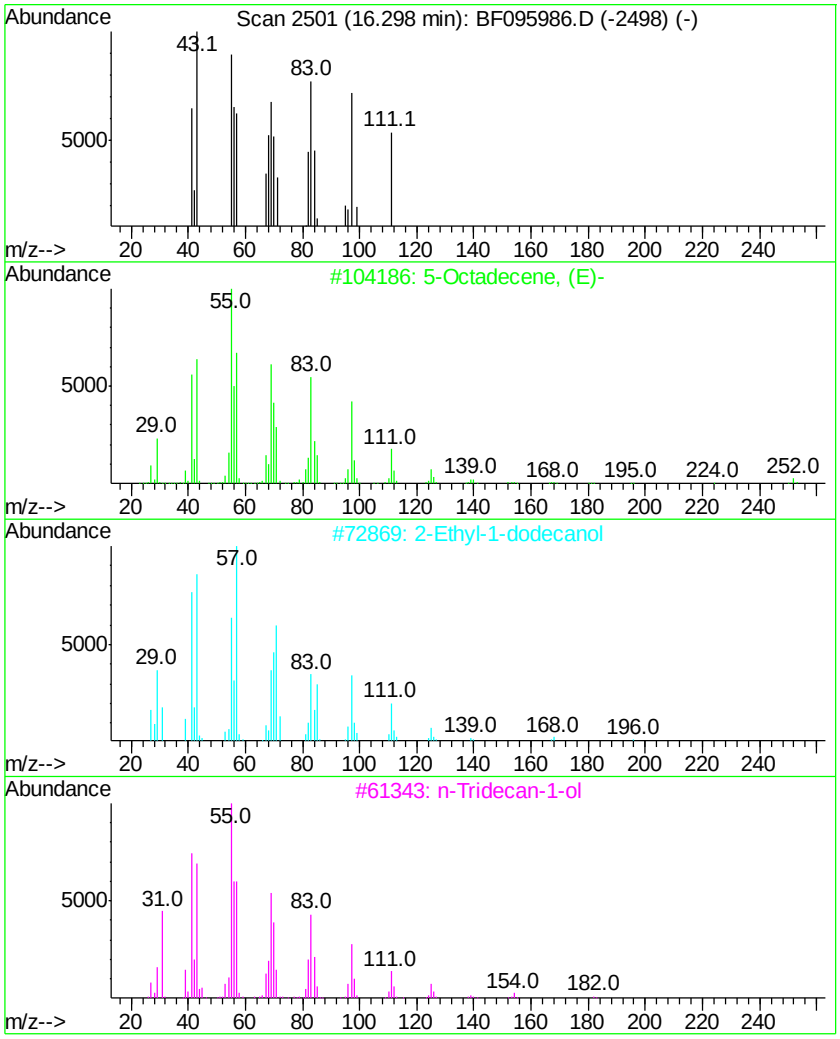
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

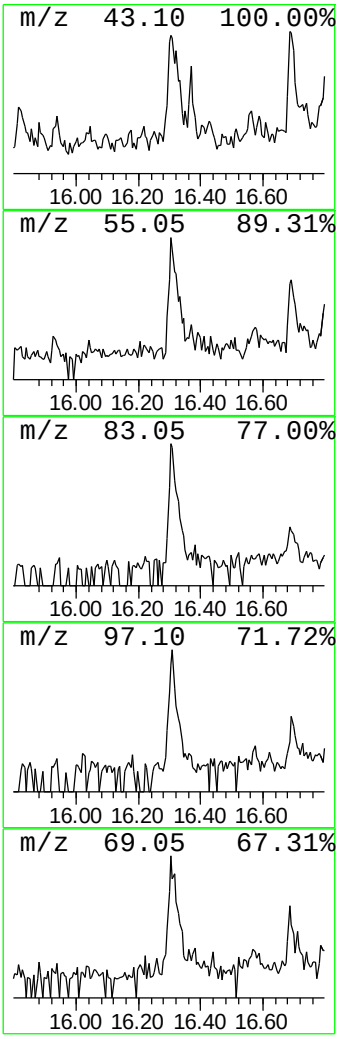
****

Peak Number 5 5-Octadecene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	2.36 ng	49587	Phenanthrene-d10	14.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	86
2	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	47
3	n-Tridecan-1-ol	200	C13H28O	000112-70-9	47
4	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	38
5	2-Hexenal, (E)-	98	C6H10O	006728-26-3	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

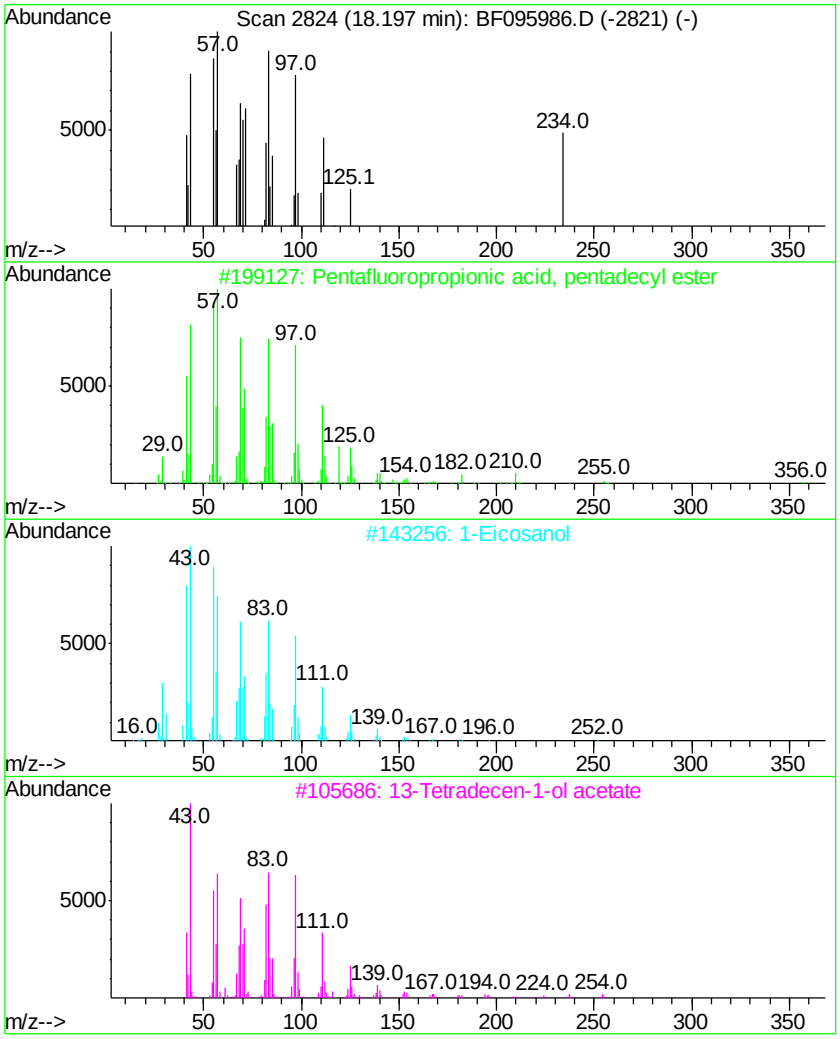
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

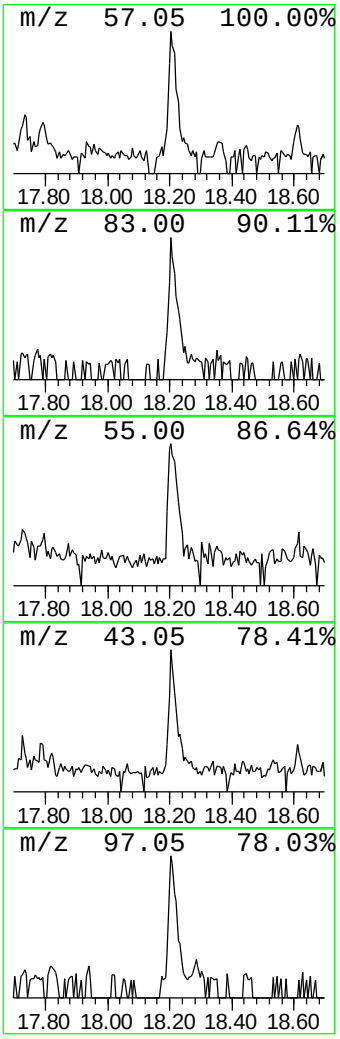
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.20	2.59 ng	53789	Chrysene-d12	18.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
2	1-Eicosanol	298	C20H42O	000629-96-9	87
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	86
4	1-Heneicosanol	312	C21H44O	015594-90-8	83
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

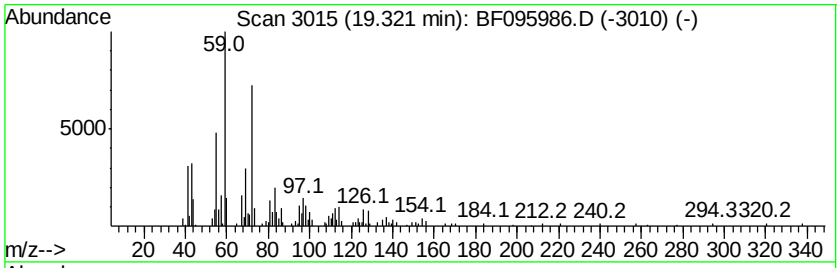
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

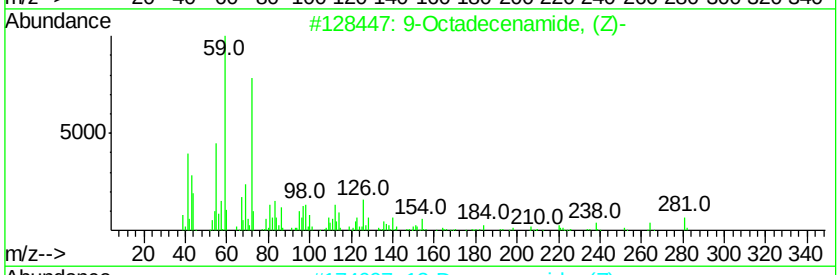
****

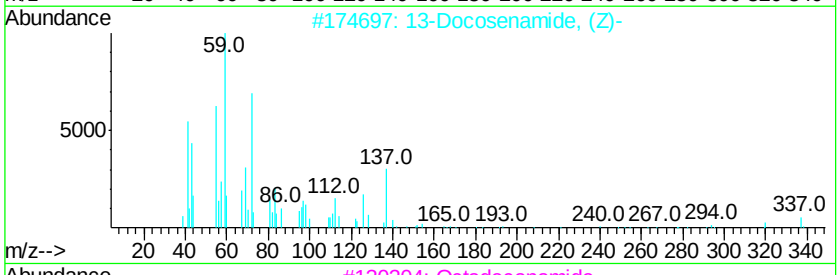
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

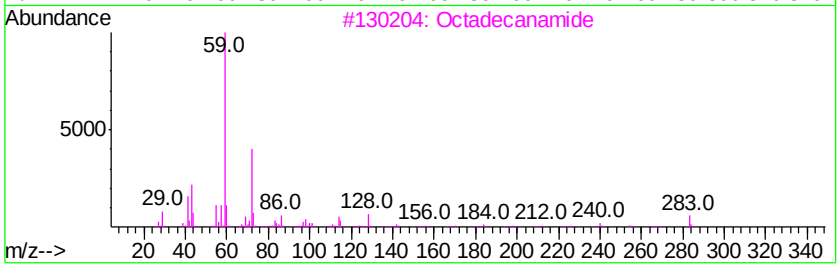
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	12.06 ng	223175	Perylene-d12	19.96

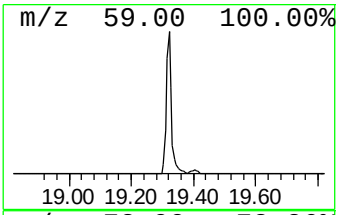
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3	Octadecanamide	283	C18H37NO	000124-26-5	53
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	47
5	2-Methyl-2-decanol	172	C11H24O	003396-02-9	43

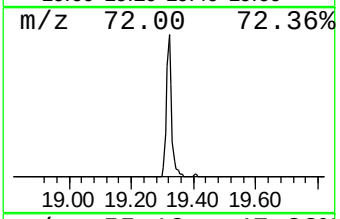


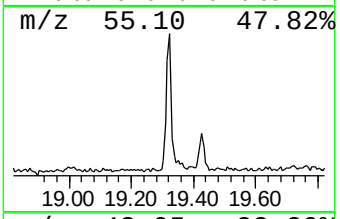


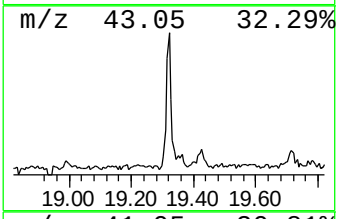


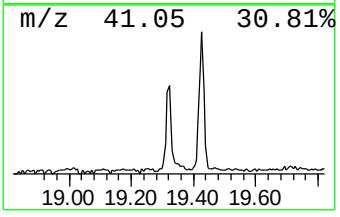












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Acq On : 17 Jun 2017 8:45
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Sample : I3688-13
Misc :
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Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

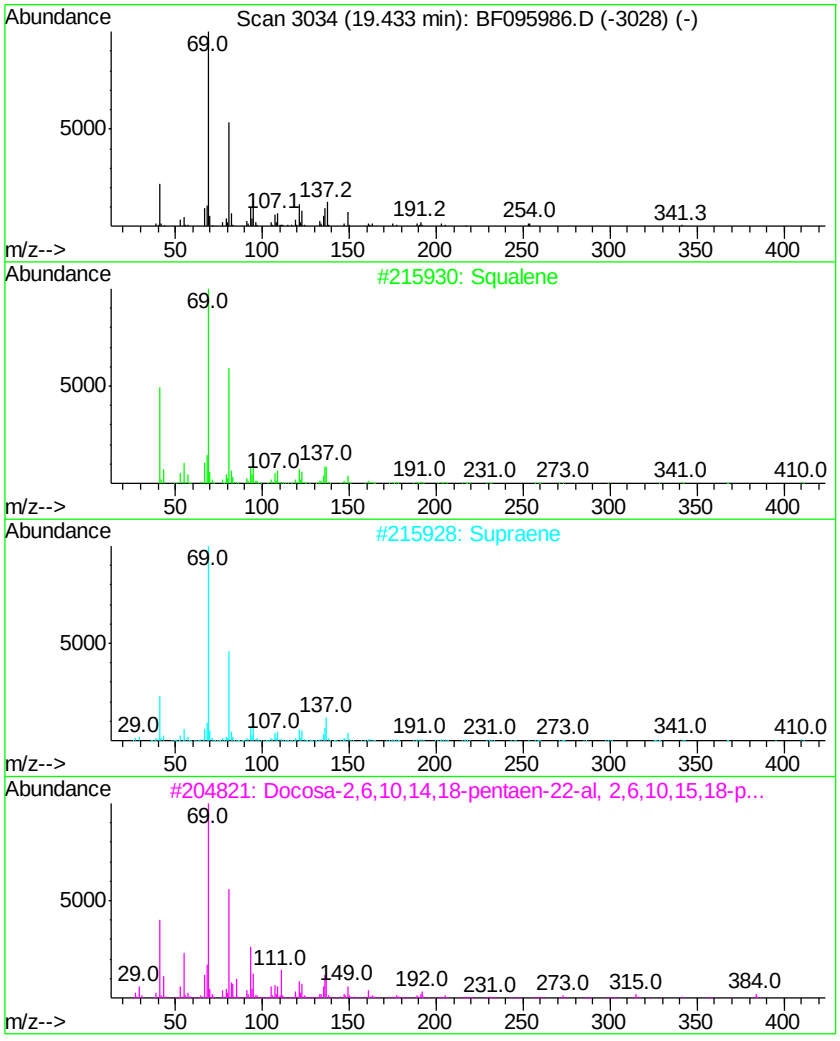
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

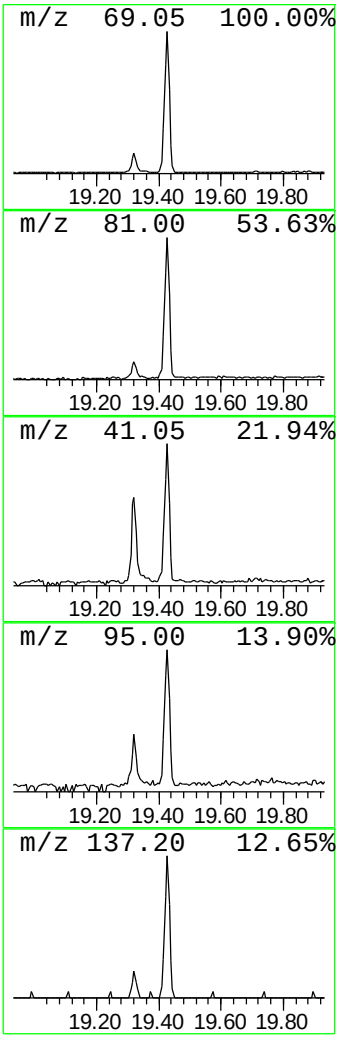
****

Peak Number 8 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	13.86 ng	256659	Perylene-d12	19.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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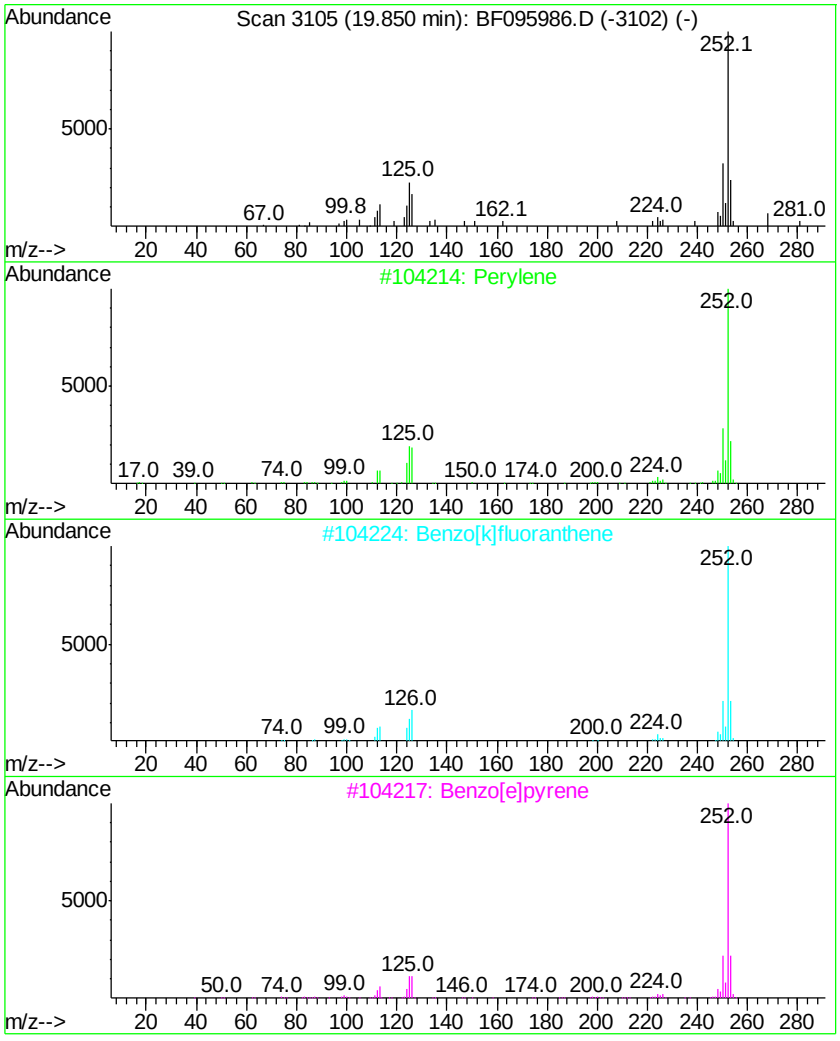
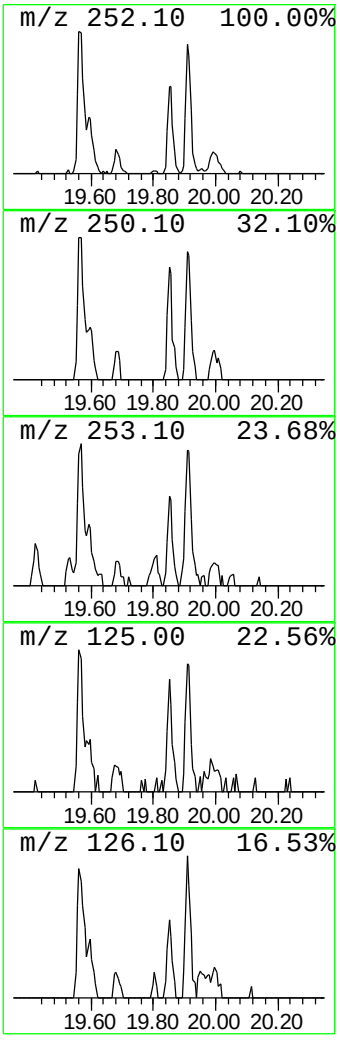
Peak Number 9 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.85	2.42 ng	44788	Perylene-d12	19.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061617\
Data File : BF095986.D
Acq On : 17 Jun 2017 8:45
Operator : SJ/MA
Sample : I3688-13
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G13-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.52	9.1	ng	156726	1	7.32	342872	20.0
unknown6.98	6.98	113.2	ng	1940160	1	7.32	342872	20.0
n-Hexadecanoic acid	15.59	5.8	ng	121560	4	14.57	421097	20.0
5-Octadecene, (E)-	16.30	2.4	ng	49587	4	14.57	421097	20.0
Pentafluoropropio...	18.20	2.6	ng	53789	5	18.29	415646	20.0
9-Octadecenamide,...	19.32	12.1	ng	223175	6	19.96	370236	20.0
Squalene	19.43	13.9	ng	256659	6	19.96	370236	20.0
Perylene	19.85	2.4	ng	44788	6	19.96	370236	20.0